Öğüt, Chelikowsky, and Louie Reply: Godby and White point out [1] that the standard procedure of estimating the quasiparticle gap for an n-electron Si quantum dot using ground state total energies as

$$\varepsilon_g^{\mathrm{qp}} = E(n+1) + E(n-1) - 2E(n) \qquad (1)$$

will not approach the quasiparticle energy gap of bulk silicon (1.2 eV) in the limit of very large clusters, when the calculations are performed within the local density approximation (LDA). They note that in the infinite cluster limit, the energies calculated using Eq. (1) should approach the LDA eigenvalue band gap (or HOMO-LUMO gap) $\varepsilon_g^{\mathrm{HL}}$, hence, the correction $\Sigma = \varepsilon_g^{\mathrm{qp}} - \varepsilon_g^{\mathrm{HL}}$ will be zero. We are well aware of this limitation of LDA. However, our original paper [2] makes no suggestion that using Eq. (1) within LDA for quantum dots much larger than the ones considered would be valid. The focus of our work is on the quasiparticle and optical gaps of Si nanocrystals with diameters $d < 2.8$ nm. In this range, Eq. (1) is a good estimate of the quasiparticle gap, even when the total energies are calculated using LDA. The concern expressed in the Comment is a misinterpretation of a minor point of our paper in which the calculated gaps and self-energy corrections were extrapolated to larger clusters using the known bulk limits. Such extrapolations were *not* meant to imply that the correct bulk limits for the quasiparticle gaps would be approached, if one were able to keep on using Eq. (1) within LDA for larger and larger clusters. Rather, we viewed them as a convenient way of extrapolating the good estimates of the calculated gaps and corrections to system sizes which are not amenable to *ab initio* calculations.

The important issue is how accurate Eq. (1) is in capturing the correction to $\varepsilon_g^{\mathrm{HL}}$. To gain insights into this problem, we compared the calculated $\varepsilon_g^{\mathrm{HL}}$ and $\varepsilon_g^{\mathrm{qp}}$ gaps [using Eq. (1)] with experiment for a few small hydrogenated Si clusters. For example, the calculations for SiH_4 yield values of 8.0 eV and 12.6 eV for $\varepsilon_g^{\mathrm{HL}}$ and $\varepsilon_g^{\mathrm{qp}}$, respectively, while the experimental values are 12.4 and 12.8 eV [3]. For the case of Si_2H_6, the calculated $\varepsilon_g^{\mathrm{HL}} = 6.5$ eV is also improved substantially to a quasiparticle gap of $\varepsilon_g^{\mathrm{qp}} = 10.6$ eV, in very good agreement with the experimental values of 10.5 and 10.7 eV [3]. These calculations show that quasiparticle gaps calculated using Eq. (1) within LDA accounts for most of the self-energy correction to the HOMO-LUMO gap on small hydrogenated Si clusters. Hence, Eq. (1) presents a simple and accurate way of calculating *ab initio* quasiparticle energies. Although the infinite cluster limit of Eq. (1) will yield $\varepsilon_g^{\mathrm{HL}}$, Σ is still substantial, being ≈ 1.1 eV, for the largest cluster $Si_{525}H_{276}$ calculated. Therefore, we do not agree with the suggestion by Godby and White that the quasiparticle gaps and optical gaps in Ref. [2] should all be increased by approximately 0.68 eV.

Finally, we would like to examine the analysis of the data for the ΔLDA correction in the Comment, which the authors presented to confirm their theoretical analysis. In particular, the authors fitted our 12 calculated data points for the self-energy correction as read from Fig. 1 of Ref. [2] to a function of the diameter as $\Sigma(d) = K + Ad^{-p}$ to find values of $K = 0.12$ eV and $p = 0.92$. They claimed that the fit obtained this way by treating K as a free parameter, instead of constraining it to 0.68 eV, is twice as good, as measured by χ^2. This result is hardly surprising. A fit to just 12 data points with three free parameters is bound to be better than with two free parameters. There is even a more important issue in using the fits suggested in the Comment to find the bulk limit of Σ: Extrapolating the 12 self-energy corrections from a size regime of a few nanometers (less than a thousand atoms) to the bulk limit, which would correspond to millions or billions of atoms, simply does not make sense from a statistical analysis point of view. Slight changes in the 12 calculated values in the $1 < d < 3$ nm size regime will have substantial effects in the calculated bulk limit of the self-energy. Therefore, from an inadequate amount of data, it is quite misleading to use any kind of least-squares fitting to confirm a value for the bulk limit of Σ.

In summary, while we agree with and are well aware of the point of the Comment, we stress that (i) it results from a misinterpretation of a minor point of our paper, and the recognition of this point does not change any of the main results presented; (ii) as a side product of the calculated results, Ref. [2] simply provides convenient formulas to extrapolate the quasiparticle gaps and self-energy corrections to a larger size regime; and (iii) the fitting procedure in the Comment cannot be used to deduce the large-size limit of the calculated corrections.

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